

Conventions, Accuracy Metrics, Classification, Regression

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Outline

1. Introduction and Demos
2. Machine Learning Fundamentals
3. First ML Example: Tomato Quality Prediction
4. Classification vs Regression
5. Classification Metrics
6. Regression Metrics
7. Data Visualization and Baselines
8. Summary and Key Takeaways

Demo

Comet browser and automation of tasks

Revision: What is Machine Learning

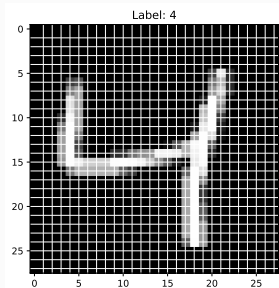
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Let us work on the digit recognition problem.

Notebook: rule-based-vs-ml.html



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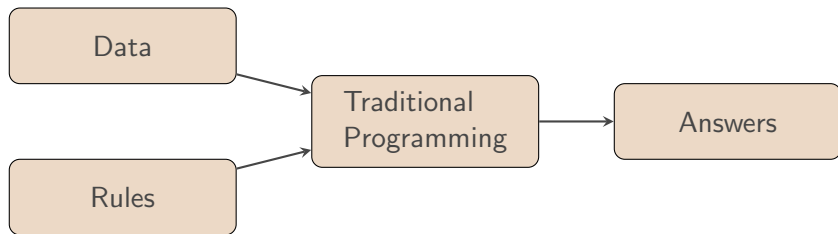
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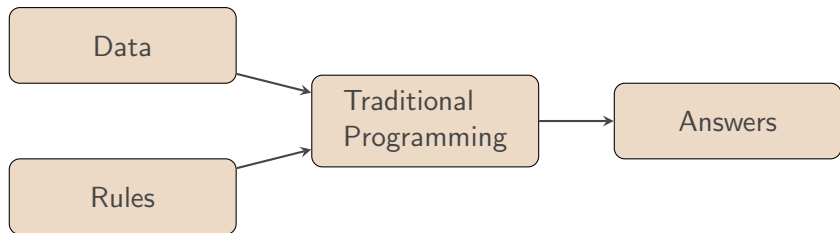
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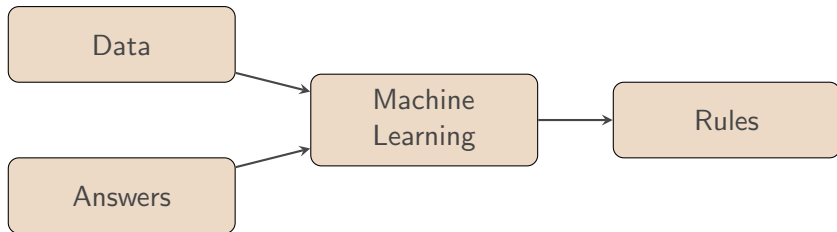
Traditional Programming vs Machine Learning



Traditional Programming



Machine Learning



Revision: What is Machine Learning

“A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T , as measured by P , improves with experience E .” - Tom Mitchell

First ML Task: Grocery Store Tomato Quality Prediction

Problem statement: You want to predict the quality of a tomato given its visual features.

Dataset

Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

Dataset

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Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

- Size
- Colour

Dataset

Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

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Dataset

Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

- Size
- Colour
- Texture

Sample Dataset

Here is our example dataset with tomato features:

Sample	Colour	Size	Texture	Condition
1	Orange	Small	Smooth	Good
2	Red	Small	Rough	Good
3	Orange	Medium	Smooth	Bad
4	Yellow	Large	Smooth	Bad

Pop Quiz #1

Quick Quiz 1

Is the sample number a useful feature for predicting quality of a tomato?

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Is the sample number a useful feature for predicting quality of a tomato?

Answer: Usually no! Sample numbers are typically arbitrary identifiers and not meaningful features. Let us remove it.

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When could sample number be useful?

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Quick Quiz 1

When could sample number be useful?

In some cases, the sample number might be useful for tracking or auditing purposes. E.g. if some trucks are delayed during delivery, the sample number could help identify which batch of tomatoes was affected.

Useful Features

Useful Features

Let us modify our data table for now.

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
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Training Set

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The training set consists of two parts:

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The training set consists of two parts:

1. Features (Input Variables)
2. Output or Response Variable

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Computers work with numbers! We need to encode categorical data numerically (one-hot encoding):

C0	C1	S0	S1	T0	T1	Good?
0	0	1	0	1	0	1
0	1	1	0	0	1	1
0	0	0	1	1	0	0
1	0	0	0	1	0	0

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Orange=00, Red=01, Yellow=10; Small=10, Medium=01, Large=00; Smooth=10, Rough=01; Good=1, Bad=0
More details on encoding later!

Data Matrix

C0	C1	S0	S1	T0	T1	Good?
0	0	1	0	1	0	1
0	1	1	0	0	1	1
0	0	0	1	1	0	0
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Data Matrix

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0	0	1	0	1	0	1
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We call this data matrix \mathbf{X} , and the complete dataset \mathcal{D} :

1. Feature matrix ($\mathbf{X} \in \mathbb{R}^{n \times d}$) containing data of n samples each of which is d dimensional.

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2. Output vector ($\mathbf{y} \in \mathbb{R}^n$) containing output variable for n samples.

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For this example: $n = 4$ (samples), $d = 6$ (features after one-hot encoding)

Mathematical Notation Convention

Important: Mathematical Notation Convention

Matrices use **bold uppercase** (\mathbf{X}), vectors use **bold lowercase** (\mathbf{y}), scalars use regular letters (n, d)

Example: Examples from Our Tomato Dataset

- **Scalars:** $n = 4$ (samples), $d = 6$ (features), $y_1 = 1$

Convention: We write $[a, b, c]^T$ instead of $\begin{bmatrix} a \\ b \\ c \end{bmatrix}$ to save space

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For this example: $n = 4$, $d = 6$, so $\mathbf{X} \in \mathbb{R}^{4 \times 6}$ and $\mathbf{y} \in \mathbb{R}^4$

Prediction Task

Estimate condition for unseen tomatoes (#5, 6) based on data set.

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Red	Large	Rough	?
Orange	Large	Rough	?

Testing Set

Testing set is similar to training set, but, does not contain labels for output variable.

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Training set used to learn f , **Test set** for predictions

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Important: Key Question

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Key Points

Generalisation = Performance on **unseen data** from the same distribution as training data

Sample vs Population: A Simple Example

Example: Tomato Farm: 10,000 tomatoes ready for harvest

- **Population:** All 10,000 tomatoes

Key Challenge: Will your 100 tomatoes represent all 10,000?
What if you only picked from one corner?

ML Connection: Training/test sets are samples from a larger population of all possible data

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From Tomatoes to Machine Learning

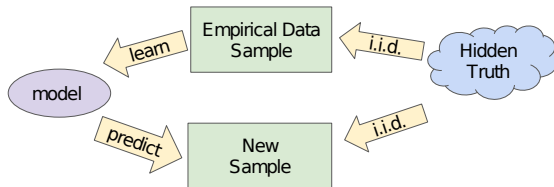


Image courtesy Google ML crash course

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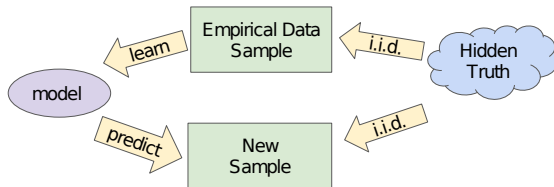


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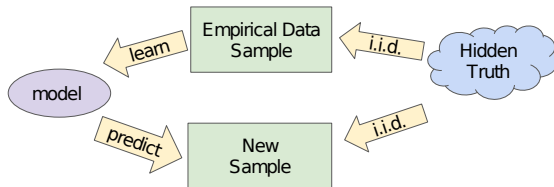


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From Tomatoes to Machine Learning

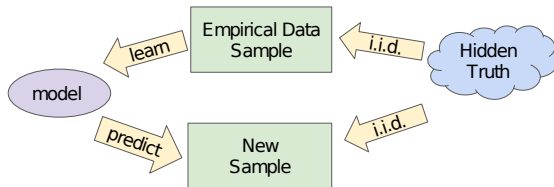


Image courtesy Google ML crash course

The ML Connection:

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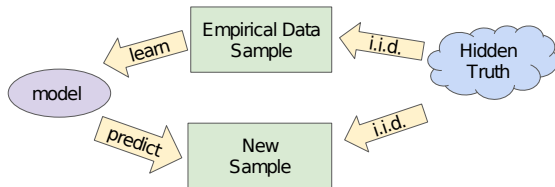


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The ML Connection:

- **Population:** All possible tomato data (past, present, future)
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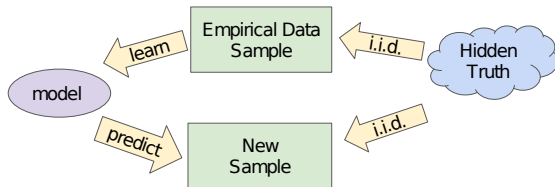


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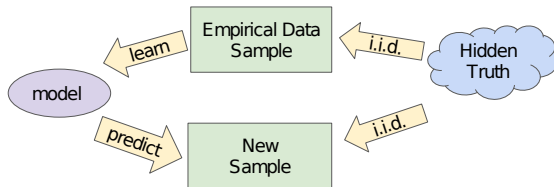


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The ML Connection:

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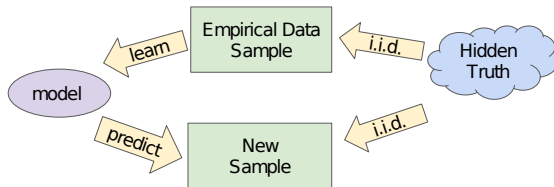


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- **Population:** All possible tomato data (past, present, future)
- **Training set:** Our 4 tomato samples (like picking from one area)
- **Test set:** 2 new samples (like picking from another area)

Generalisation goal: Will our model work on *all future tomatoes*, not just our small samples?

Second ML Task: Campus Energy Prediction

Regression Problem: Predicting continuous energy consumption (kWh)

Key factors: # People, Temperature

# People	Temp (°C)	Energy (kWh)
4000	30	30
4200	30	32
4200	35	40
3000	20	?
1000	45	?

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Difference from tomatoes: Energy is *continuous*, not categories

Classification vs Regression

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 - How much rainfall will fall?

Pop Quiz #2

Quick Quiz 2

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- c) Predicting house prices
- d) Determining if a tumor is malignant or benign

Pop Quiz #2 - Answer

Answer: c) House prices are continuous values - that's regression!

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If our model predicts 5 tomatoes correctly and 3 incorrectly, is that good or bad? We need metrics!

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Coming up: Different metrics for classification vs regression problems

Back to Our Tomato Example: How Did We Do?

Let's say we trained our model and tested it on 5 new tomatoes:

#	Actual	Predicted
1	Good	Good
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Questions:

- How many did we get right? How many wrong?
- Is 3 out of 5 correct “good enough”?
- What if getting a bad tomato wrong is worse than getting a good tomato wrong?

Organizing Our Results

Let's organize the predictions in a simpler way:

Model Predicted (\hat{y})	Actually Was (y)
Good	Good
Good	Good
Good	Bad
Good	Bad
Bad	Bad

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Each row = one tomato's result

Goal: Create systematic ways to measure performance from these comparisons

Converting to Numbers for Computation

Remember: Computers work with numbers! Let's encode our categories:

Example: Binary Encoding

Bad = 0, **Good** = 1

Now our results become:

$$\begin{matrix} & \text{Predicted } (\hat{y}) \\ \left(\begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 0 \end{array} \right) \end{matrix}$$

$$\begin{matrix} & \text{Ground Truth } (\mathbf{y}) \\ \left(\begin{array}{c} 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{array} \right) \end{matrix}$$

Ground Truth = The correct answers (what actually happened)

Accuracy: Measuring Overall Performance

How many predictions did we get exactly right?

	Predicted (\hat{y})	Ground Truth (y)
✓	1	1
✓	1	1
	1	0
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For our example: $\text{Accuracy} = \frac{3}{5} = 0.6$ or 60%

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$$\text{Accuracy} = \frac{\sum_{i=1}^n \mathbf{1}[y_i = \hat{y}_i]}{n}$$

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- Both notations are mathematically equivalent and commonly used in ML literature

Two Views: Predictions vs Confusion Matrix

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Confusion Matrix

		Bad	Good
Pred	Bad	1	0
	Good	2	2

Confusion Matrix: Understanding the Four Outcomes

		Ground Truth	
		Positive	Negative
Predicted	Positive	TP	FP
	Negative	FN	TN

Definition: Four Outcomes

- **TP (True Positive):** Correctly predicted positive

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Confusion Matrix: Precision Focus

Confusion Matrix		Ground Truth		Row Totals
Predicted		Positive	Negative	
	Positive	TP	FP	TP + FP
	Negative	FN	TN	FN + TN
		TP + FN	FP + TN	Total

Example: Focus: Predicted Positives

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

“Of all predicted positives, how many were actually positive?”

Confusion Matrix: Recall Focus

Confusion Matrix		Ground Truth		Row Totals
Predicted		Positive	Negative	
	Positive	TP	FP	TP + FP
	Negative	FN	TN	FN + TN
		TP + FN	FP + TN	Total

Example: Focus: Actual Positives

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

“Of all actual positives, how many did I catch?”

When Classes Are Imbalanced

Many datasets have unequal class distributions!

Example: Example: Medical Screening

Out of 1000 patients tested:

- **990** patients are healthy (negative class)

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Smart Classifier

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- Precision: $\frac{8}{48} \approx 16.7\%$
- Recall: $\frac{8}{10} = 80\%$
- Accuracy: $\frac{8+950}{1000} = 95.8\%$

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- May miss positives (\uparrow FN)
- Useful when FP is costly

Definition: High Recall

- Captures most positives
- Few misses (\downarrow FN)
- More false alarms (\uparrow FP)

Precision vs Recall: The Trade-off

You often can't have both high precision and high recall — improving one may reduce the other.

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Accuracy Metric: F1-Score

		Ground Truth	
		Positive	Negative
Predicted	Positive	TP	FP
	Negative	FN	TN

Example: F1-Score: Balancing Precision and Recall

$$F1 = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

Accuracy Metric: Matthews Correlation Coefficient (MCC)

		Ground Truth	
		Positive	Negative
Predicted	Positive	TP	FP
	Negative	FN	TN

Example: MCC: Balanced Performance Measure

$$\text{MCC} = \frac{TP \cdot TN - FP \cdot FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}$$

MCC Comparison: Dummy vs Smart Classifier

MCC Comparison: Dummy vs Smart Classifier

Dummy Classifier

Confusion Matrix		Ground Truth	
		Pos	Neg
Pred	Pos	0	0
	Neg	10	990

$MCC = 0$ (denominator undefined; treat as 0)

MCC Comparison: Dummy vs Smart Classifier

Dummy Classifier

Confusion Matrix		Ground Truth	
		Pos	Neg
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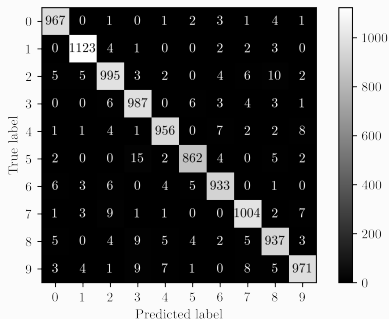
Smart Classifier

Confusion Matrix		Ground Truth	
		Pos	Neg
Pred	Pos	8	40
	Neg	2	950

$$\text{MCC} = 0 \quad (\text{denominator undefined; treat as } 0) \quad \text{MCC} = \frac{7600}{\sqrt{(48)(10)(990)(952)}} \approx \mathbf{0.26}$$

Confusion Matrix for multi-class classification

Notebook: confusion-mnist.html



Metrics for Regression: MSE & MAE

Prediction (\hat{y})	Ground Truth (y)
10	20
20	30
30	40
40	50
50	60

$$\text{Mean Squared Error (MSE)} = \frac{\sum_{i=1}^n (\hat{y}_i - y_i)^2}{n}$$

$$\text{Root Mean Square Error (RMSE)} = \sqrt{\text{MSE}}$$

Accuracy Metrics: MAE & ME

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Is there any downside with using mean error?

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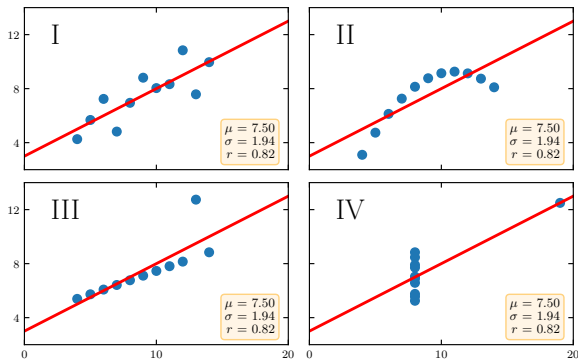
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Is there any downside with using mean error?

Errors can get cancelled out

The Importance of Plotting

Notebook: anscombe.html



Anscombe's Quartet

Dummy Baselines

Notebook: dummy-baselines.html

The Importance of Plotting

Property	Value	Across datasets
mean(X)	9	exact
mean(Y)	7.5	up to 3 decimal places
Linear regression line	$y = 3.00 + 0.500x$	up to 2 decimal places

Pop Quiz #3

Quick Quiz 3

For imbalanced datasets, which metrics should you prioritize over accuracy?

- a) Only precision

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Pop Quiz #3

Quick Quiz 3

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- a) Only precision
- b) Only recall
- c) Precision, recall, and F1-score
- d) Only confusion matrix

Pop Quiz #3 - Answer

Answer: c) Precision, recall, and F1-score give a more complete picture!

Key Takeaways

Key Points

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- **Visualization is crucial:** Always plot your data (Anscombe's Quartet lesson)
- **Use baselines:** Simple baseline models help validate your approach